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## **FINAL REPORT**

**AFOSR Grant 49620-93-1-0134**

**Cluster Ions**

**February 1, 1993 to February 1, 1996**

### **I. Abstract**

One of the truly difficult tasks in molecular science is determining experimental conformations of either highly reactive species or species that have essentially no vapor pressure at any accessible temperature. In the past three years significant progress has been made in developing methods to attack this problem using ion mobility techniques developed with support from this grant. Initial applications have been to carbon clusters, carbon metal composites, gas phase polymers, and host/guest systems. A total of 19 papers were published in peer reviewed journals, and numerous invited and contributed papers were given at conferences describing this work.

### **II. Objectives**

- A. Characterization of Gas Phase Growth Mechanisms and/or Conformations of
  - 1. Carbon Based Clusters
  - 2. Semiconductor and Carbon/Metal Composite Clusters
  - 3. Polymers, Crown Ethers and other Macromolecules
- B. Development of the Methodology for Accomplishing the Objectives Listed Above

### **III. Progress**

Details of the progress made during the grant period can be found in the various annual reports and 19 papers published in peer reviewed journals. Of recent importance is the completion of the second ion chromatography instrument in Fall, 1995. This instrument has been thoroughly tested using a simple electron impact source, and new sources are currently under development. Different projects can now be run in parallel, reducing the significant dead time in switching from project to project.

This three year grant period has been exciting, with breakthrough work being accomplished in several areas. These include fullerene formation mechanisms, metcar structures and the first matrix assisted laser desorption experiments. These latter experiments show great promise for conformational analysis of macromolecules, including polymers and biopolymers. They also allow determination of binding energies of H<sub>2</sub>O and other ligands to alkali metal cationized crown ethers and other host molecules, experiments initiated but not completed during this grant period.

#### IV. Papers Published or in Press\*

1. One- and Two-Dimensional Carbon Clusters: Isomers, Structures and Isomer Abundances, Gert von Helden, Ming-Teh Hsu, Paul R. Kemper and Michael T. Bowers, Materials Research Society, Symposium Proceedings, *Novel Forms of Carbon* **270**, 117 (1992).
2. Isomers of Small Carbon Cluster Anions: Linear Chains with up to 20 Atoms, G. von Helden, P.R. Kemper, N.G. Gotts and M.T. Bowers, *Science* **259**, 1300 (1993).
3. Do Small Fullerenes Exist Only on the Computer? Experimental Results on  $C_{20}^{+/-}$  and  $C_{24}^{+/-}$ , G. von Helden, M-T. Hsu, N.G. Gotts, P.R. Kemper and M.T. Bowers, *Chem. Phys. Lett.* **204**, 15 (1993).
4. Experimental Evidence for the Formation of Fullerenes by Collisional Heating of Carbon Rings in the Gas Phase, G. von Helden, N.G. Gotts and M.T. Bowers, *Nature* **363**, 60 (1993).
5. Annealing of Carbon Cluster Cations: Rings to Rings and Rings to Fullerenes, G. von Helden, N.G. Gotts and M.T. Bowers, *J. Am. Chem. Soc.* **115**, 4363 (1993).
6. Gas-Phase Ion Chromatography: Transition Metal State Selection and Carbon Cluster Formation, M.T. Bowers, P.R. Kemper, G. von Helden and P.A.M. van Koppen, *Science* **260**, 1446 (1993).
7. Carbon Cluster Cations with up to 84 Atoms: Structures, Formation Mechanism and Reactivity, G. von Helden, M-T. Hsu, N. Gotts and M.T. Bowers, *J. Phys. Chem.* **97**, 8182 (1993).
8.  $C_7^+$  is Cyclic: Experimental Evidence, G. von Helden, N.G. Gotts and M.T. Bowers, *Chem. Phys. Lett.* **212**, 241 (1993).
9. The Lowest Energy Structures of  $C_7^+$ ,  $C_7$  and  $C_7^-$ : An Ab Initio Study, G. von Helden, W.E. Palke and M.T. Bowers, *Chem. Phys. Lett.* **212**, 247 (1993).
10. Structures and energies of Small Carbon Clusters: What Experiment and Theory Have to Say about  $C_8^+$ ,  $C_8^+$  and  $C_{10}^+$ , G. von Helden, N.G. Gotts, W.E. Palke and M.T. Bowers, *Int. J. Mass Spectrom. Ion Proc.* **138**, 33 (1994).
11. The Structures of Small Iron-Carbon Cluster Anions. Linear to Planar to Three-Dimensional, G. von Helden, Nigel G. Gotts, P. Maitre and M.T. Bowers, *Chem. Phys. Lett.* **227**, 601 (1994).
12. Cluster Ions: Carbon, Met-cars and  $\sigma$ -Bond Activation, Michael T. Bowers, *Acct. Chem. Research*, **27**, 234 (1994).
13. Structures of Carbon Clusters from Polychlorinated Graphitic Precursors: Investigations of  $C_{12}Cl_x^+$  ( $x=0$  to 10) Using the Ion Chromatography Method, G. von Helden, E. Porter, N.G. Gotts and M.T. Bowers, *J. Phys. Chem.*, (in press).
14. Met-cars are Hollow Cage Clusters: Evidence from Ion Chromatography Experiments, S. Lee, N.G. Gotts, G. von Helden and M.T. Bowers, *Science* **267**, 999 (1995).
15. Conformation of Macromolecules in the Gas Phase: Coupling of a MALDI Source to the Ion Chromatography Technique, G. von Helden, T. Wytenbach and M.T. Bowers, *Science*, **267**, 1483 (1995).

16. Factors Affecting  $\sigma$ -Bond Activation in Simple Systems: Measurement of Experimental Binding Energies of  $\text{Fe}^+(\text{H}_2)_{1-6}$  Clusters, J.E. Bushnell, P.R. Kemper, and M.T. Bowers, *J. Phys. Chem. Z. Herman Honor Issue*, **99**, 15602 (1995).
17. Inclusion of a MALDI ion Source in the Ion Chromatography Technique: Conformational Information on Polymer and Biomolecular Ions, G. von Helden, T. Wytttenbach, and M.T. Bowers, *Int. J. Mass Spectrom. Ion Proc. Al Nier Honor Issue*, **146/147**, 349 (1995).
18. Gas Phase Conformations of  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$  and  $\text{Cs}^+$  Complexed with 18-crown-6, S. Lee, T. Wytttenbach, G. von Helden, and M.T. Bowers, *J. Am. Chem. Soc.* **117**, 10159 (1995).
19. Carbon Cluster Anions: Structure and Growth from  $\text{C}_2^-$  to  $\text{C}_{10}^-$ , N.G. Gotts, G. von Helden, and M.T. Bowers, *Int. J. Mass Spectrom. Ion Proc. David Smith Honor Issue*, **149/150**, 217 (1995).

## V. Personnel Associated with the Project

### A. Senior:

Dr. Paul Kemper	Dr. W. E. Palke
Dr. Petra van Koppen	Dr. Philippe Maitre
Dr. Nigel Gotts	Dr. Thomas Wytttenbach
Dr. Seung-Hoon Lee	

### B. Junior:

Mr. Gert von Helden	Mr. Ed Porter	Mr. John Bushnell
Mr. Ming-Teh Hsu	Mr. Doug Carlat	

## VI. Papers Presented at Meetings/Universities\*

### A. Invited Lectures

1. Symposium on Fullerenes, National ACS Meeting, Denver, CO, March, 1993
2. Symposium on New Forms of Carbon, Materials Research Society Meeting, San Francisco, CA April, 1993
3. Symposium on Fullerenes, National Electrochemical Society Meeting, Honolulu, HI, May, 1993
4. Symposium on Fullerenes, National Electrochemical Society Meeting, New Orleans, LA, October, 1993
5. Invited Participant/Lecturer, Joint US-Japan Workshop on Clusters, Hawaii, March, 1994
6. Invited Participant/Lecturer, Workshop on Carbon in the Gas Phase, Berlin, Germany, March, 1994
7. Faculty Research Lecture, UCSB, April, 1994
8. Symposium on Mass Spectrometry of Fullerenes and Related Species, National Electrochemical Society Meeting, San Francisco, CA, May, 1994
9. Air Force Contractors Meeting, Washington, DC, October, 1994
10. Plenary Lecture, West Coast Theoretical Chemistry Conference, San Diego, CA, March, 1995

11. Invited Speaker, Yamada Conference on Metallic and Semiconductor Clusters, Shimoda, Japan, May, 1995
12. Keynote Lecture, Symposium on Metal Ion Chemistry, American Society for Mass Spectrometry, Atlanta, GA, May, 1995
13. Invited Speaker, ASMS Asilomar Conference on the Challenge of High Mass Ions, Pacific Grove, CA, September, 1995
14. Invited Speaker, International Symposium on the Science and Technology of Atomically Engineered Materials, Richmond, VA, November, 1995
15. Plenary Lecture, ASMS Sanibel Conference on Metal Containing Ions, Sanibel Island, FL, January, 1996

**B. Contributed Papers**

1. Presented two papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, February 1993
2. Presented two posters, Gordon Conference on Structures, Energetics and Dynamics of Gas Phase Ions, Ventura, CA, March 1993
3. Presented three papers, American Society for Mass Spectrometry, San Francisco, CA, June 1993
4. Presented poster, AFOSR Contractors Meeting, Irvine, CA, November 1993
5. Presented four papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, January, 1994
6. Presented six papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, January 1995
7. Presented four posters, Gordon Research Conference on the Structure, Energetics and Dynamics of Gaseous Ions, Ventura, CA, February, 1995
8. Presented poster, American Society for Mass Spectrometry, Atlanta, GA, May, 1995
9. Presented four papers, West Coast Ion Chemistry Conference, Lake Arrowhead, CA, January 1996

**C. Seminars at Universities**

1. University of Wisconsin at Madison, November, 1992
2. University of California at Irvine, November, 1992
3. Westmont College, Montecito, CA, December, 1992
4. University of Warwick, Coventry, U.K., December, 1992
5. University of Sussex, Brighton, U.K., December, 1992
6. University of California at Davis, February, 1993
7. University of Colorado at Boulder, April, 1993
8. University of Nevada at Las Vegas, June, 1993
9. University of Georgia at Athens, October, 1993
10. First "Dow Lecturer", University of Minnesota, Minneapolis, MN, May, 1994
11. University of California at Berkeley, September, 1994
12. Yale University, October, 1994
13. University of Illinois, Urbana, IL, April, 1995

**D. Other**

1. Vice Chair, Gordon Conference on the Structures, Energetics and Dynamics of Gaseous Ions, Ventura, CA, February, 1993
2. Presented Faculty Research Lecture, University of California, Santa Barbara, CA, April, 1994
3. Chair, Gordon Conference on the Structures, Energetics and Dynamics of Gaseous Ions, Ventura, CA, February, 1995
4. Chair, Session on "Metal-Metal Bonding from Surfaces to the Gas Phase", ACS Meeting, Anaheim, CA, April, 1995

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